Konsep Fundamental TEKNOLOGI PEMBAKARAN - 2

COMBUSTION TECHNOLOGY & THERMAL ANALYSIS

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SYLLABUS

- 1. Dasar-dasar Teknik Pembakaran (150')
- 2. Konsep Fundamental Kimia Sistem Pembakaran (2x150')
- 3. Konsep Perpindahan Panas dalam Sistem pembakaran (150')
- 4. Flame Impingement (150')
- 5. Perancangan Sistem Burner (2x150')
- 6. Troubleshooting Sistem Pembakaran (150')
- 7. Bahan Bakar untuk Proses Pembakaran (2x150')
- 8. Permodelan Proses Pembakaran (2x150')
- 9. Pengendalian Proses Pembakaran (150')
- 10. Keselamatan Proses Dalam Sistem Pembakaran (2x150')
- 11. Sistem Flare di Teknologi Pembakaran (150')

SUB-STOICHIOMETRIC COMBUSTION

- The concept of excess air presumes air in addition to that required for combustion.
- However, if one does not provide enough air, combustion may still continue, generating large quantities of CO and combustibles. ➔ called: **substoichiometric combustion**
- **Process heaters** and **boilers** should NEVER be operated in this mode
- Suddenly adding air to such a hot mixture could result in **explosion**.
- Because substoichiometric combustion may have deadly consequences, it is useful to consider the process, observe its features, and learn to avoid it.

Expression of Substoichimetric

- The stoichiometric ratio, Φ, is a fuel:air ratio (.

$$\Phi = 1/(1+\varepsilon)$$

$$\varepsilon = (1-\Phi)/\Phi$$

- Therefore:

$$CH_x + (1+\varepsilon)(1+x/4)[O_2 + 79/21\ N_2] \rightarrow CO_2 + x/2\ H_2O + \varepsilon(1+x/4)\ O_2 + (1+x/4)(1+\varepsilon)(79/21)\ N_2$$

$$CH_x + a[O_2 + 79/21\ N_2] \rightarrow b\ CO + (1-b)\ CO_2 + (x-c)/2\ H_2 + c/2\ H_2O + a\ 79/21\ N_2$$

- where a, x are specified and b, c are unknown having the relation $2a = 2 - b + c/2$.
- ε, fraction of excess air

EQUILIBRIUM AND THERMODYNAMICS

- The water gas shift reaction:

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

- When the rate of the forward reaction equals that of the reverse, the process is in dynamic equilibrium.
- Equilibrium is characterized by the following relation:

$$K = [CO_2][H_2]/[CO][H_2O]$$

- For substoichiometric combustion, it will be useful to define the following quantities: α = [H2]/[H2O], β = [CO]/[CO2], then K = α / β.

SUBSTOICHIOMETRIC COMBUSTION REVISITED

- Solving the mass balance for C, H, and oxygen, in turn for α and β, and using the relation K = α/β, one obtains the following equations:

$$CH_x + \frac{1}{2}\left[\frac{2+\beta}{1+\beta} + \frac{x}{2(1+\beta K)}\right]\left(O_2 + \frac{79}{21}N_2\right) \rightarrow$$

$$\left(\frac{1}{1+\beta}\right)CO_2 + \left(\frac{\beta}{1+\beta}\right)CO + \frac{1}{2}\left(\frac{x}{1+\beta K}\right)H_2O$$

$$+\frac{1}{2}\left(\frac{\beta K x}{1+\beta K}\right)H_2 + \left(\frac{79}{21}\right)\left(\frac{1}{2}\right)\left[\frac{2+\beta}{1+\beta} + \frac{x}{2(1+\beta K)}\right]N_2$$

- Solve the equation:

$$a = \frac{1}{\Phi}\left(1 + \frac{x}{4}\right) = \frac{1}{2}\left[\frac{2+\beta}{1+\beta} + \frac{x}{2(1+\beta K)}\right]$$

- Therefore:

$$\Phi = \frac{(x+4)(1+\beta)(1+\beta K)}{2(2+\beta)(1+\beta K)+x(1+\beta)}$$

- Solving for the species as a function of β gives:

$$TWP = 1+\frac{x}{2}+\frac{79}{21}\left[\frac{1}{1+\beta}+\frac{\beta}{2(1+\beta)}+\frac{x}{4(1+\beta K)}\right]$$

$$TDP = 1+\frac{1}{2}\left(\frac{\beta K x}{1+\beta K x}\right)+\frac{79}{21}\left[\frac{1}{1+\beta}+\frac{\beta}{2(1+\beta)}+\frac{x}{4(1+\beta K)}\right]$$

$$f_{O_2,wet}=0 \qquad f_{O_2,dry}=0$$

$$f_{CO_2,wet}=\frac{1}{TWP}\left(\frac{1}{1+\beta}\right) \qquad f_{CO_2,dry}=\frac{1}{TDP}\left(\frac{1}{1+\beta}\right)$$

$$f_{CO,wet}=\frac{1}{TWP}\left(\frac{\beta}{1+\beta}\right) \qquad f_{CO,dry}=\frac{1}{TDP}\left(\frac{\beta}{1+\beta}\right)$$

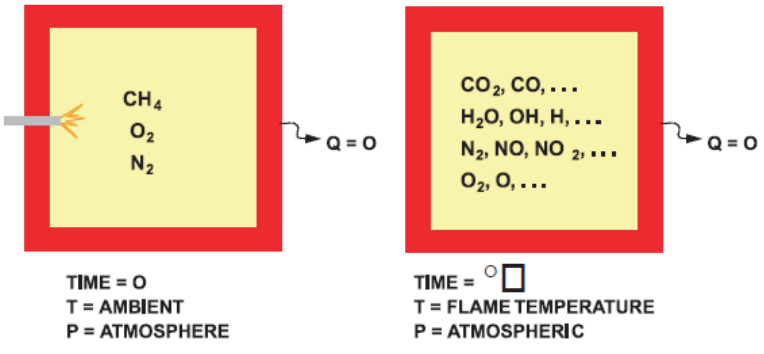
$$f_{H_2O,wet}=\frac{1}{2\,TWP}\left(\frac{x}{1+\beta K}\right)$$

$$f_{H_2,wet}=\frac{1}{2\,TWP}\left(\frac{\beta K x}{1+\beta K}\right) \qquad f_{H_2,dry}=\frac{1}{2\,TDP}\left(\frac{\beta K x}{1+\beta K}\right)$$

$$f_{N_2,wet}=\frac{79}{21}\frac{1}{2\,TWP}\left[\frac{2+\beta}{1+\beta}+\frac{x}{2(1+\beta K)}\right]$$

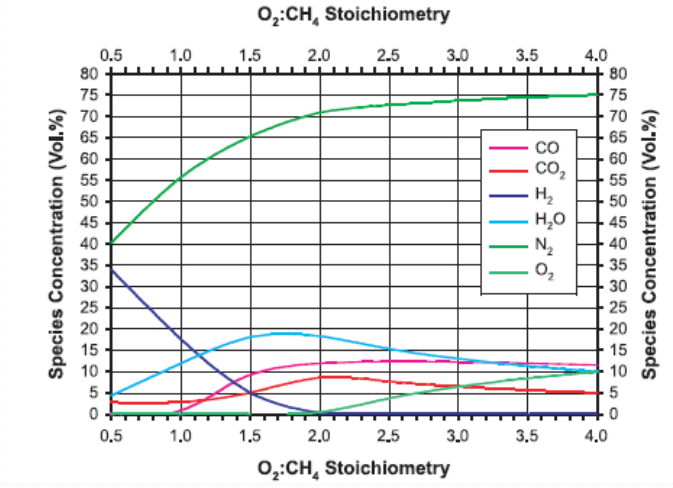
$$f_{N_2,dry}=\frac{79}{21}\frac{1}{2\,TDP}\left[\frac{2+\beta}{1+\beta}+\frac{x}{2(1+\beta K)}\right]$$

Adiabatic equilibrium reaction process.



- Many species are then present after the reaction is completed.
- The exact composition depends on the ratio of the fuel to air.
- For example, if not enough air is present, then CO will be generated. If sufficient air is present, then little or no CO will be present.

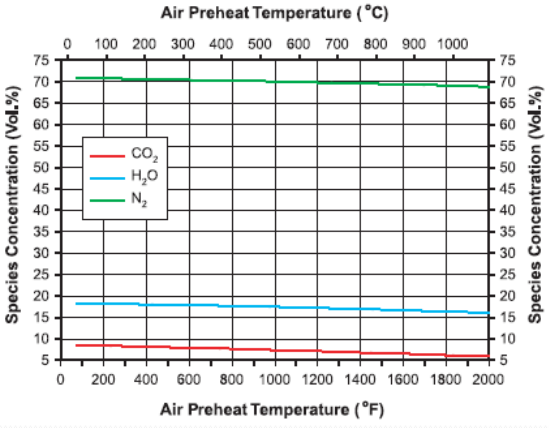
- Adiabatic equilibrium calculations for the predicted gas composition as a function of the O2:CH4 stoichiometry



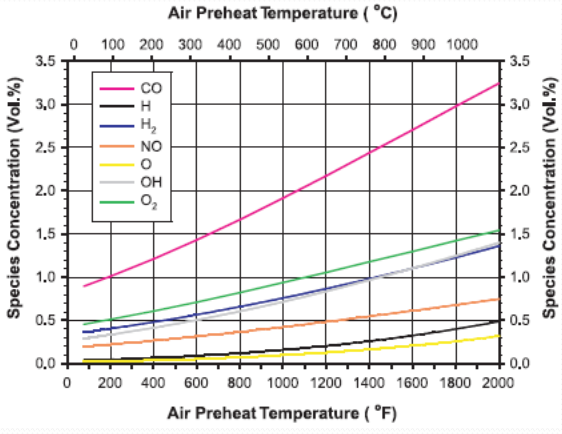
- For methane, the **stoichiometric O2:CH4 ratio** for theoretically perfect combustion is 2.0
- Stoichiometries **less than 2.0 are fuel rich**, as insufficient oxygen is present to fully combust the fuel.
- Stoichiometries **greater than 2.0 are fuel lean**, as excess oxygen is present.
- This figure shows that the exhaust product composition is highly dependent on the ratio of the fuel to the oxidizer.

Air Preheat Effect

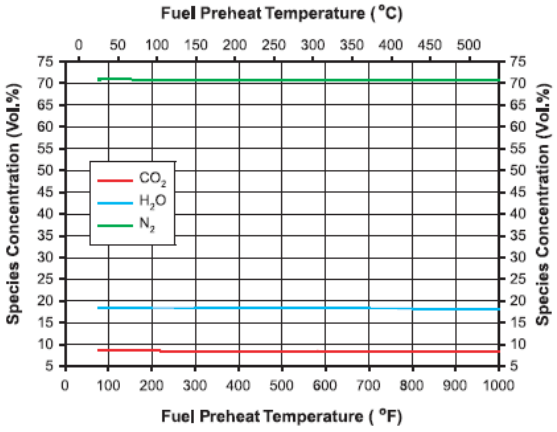
- Adiabatic equilibrium stoichiometric calculations for the predicted gas composition of the major species as a function of the **air preheat temperature for air/CH_4 flames**, where the CH_4 is at ambient temperature and pressure



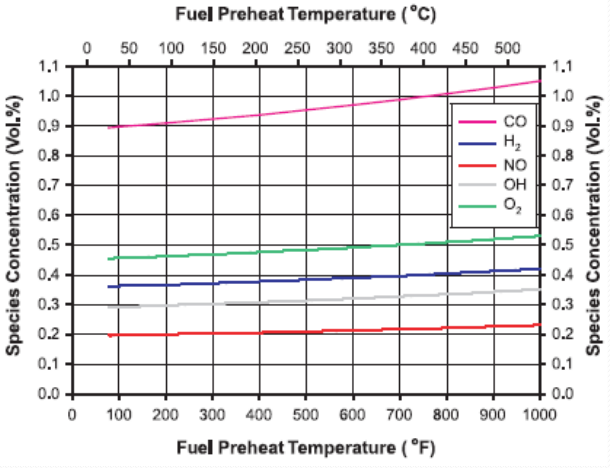
- The predicted minor species in the exhaust gas for the same reaction of ambient temperature methane with preheated air.
- This graph shows that there is a dramatic **increase in all the minor** species as the **air preheat temperature increases**. This is due to **chemical dissociation**



- **The predicted major species in the exhaust products for the combustion of preheated methane with ambient air.**
- There is **very little change in the species concentration with fuel preheat**.
- Note that higher fuel preheat temperatures present safety problems because of the auto-ignition temperature of methane, which is approximately 1200°F (650°C) in air.



- The predicted **minor species concentrations increase with fuel preheat temperature**:

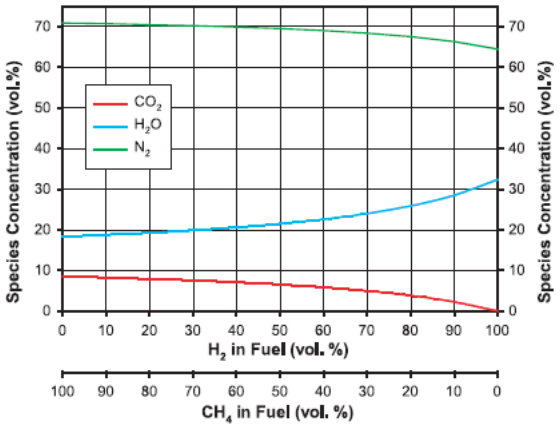


Fuel Blend Effects

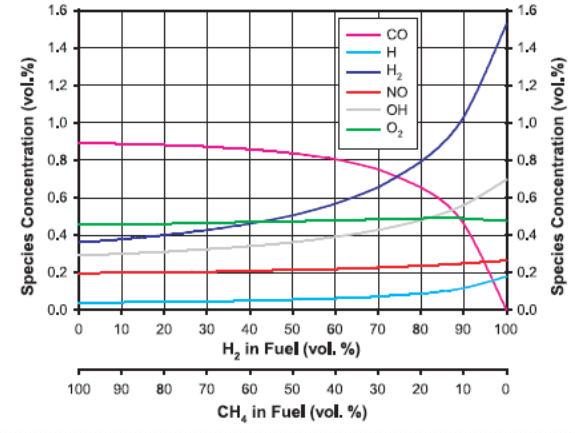
- The predicted major species for the combustion of air with fuel blends consisting of H2 and CH4

CO2 and N2 decline and H2O increases as the H2 content in the fuel increases.

It is important to note that the species concentrations are not linear functions of the blend composition, where the change occurs more rapidly at higher H2 compositions



- Plot of the **predicted minor species as functions of the H2/CH4 fuel blend**.
- This graph also shows strong nonlinearities as the H2 content increases:



- **Real combustion processes are not adiabatic**, as the whole intent is to transfer heat from the flame to some type of load.
- The amount of heat lost from the process determines the **temperature of the exhaust gases**.
- The **higher the heat losses** from the flame, the **lower the exhaust gas temperature**.

COMBUSTION KINETICS

- The **actual combustion mechanism is quite complex**, involving very short-lived species that do not survive much beyond the flame.
- For example, the simplest system — **hydrogen combustion** — comprises about 20 elemental reactions.
- **Elemental reactions denote the actual species involved in the reaction**
- M refers to Reactor wall
- **Higher hydrocarbons and more comple**

mixtures require even more reactions.

- Fortunately, the net reaction is enough

for most purposes

$$2[H_2 + M = 2H + M]$$

$$2[H + O_2 = OH + O]$$

$$O + O + M = O_2 + M$$

$$2[H + OH + M = H_2O + M]$$

$$\text{Net}: \quad 2H_2 + O_2 \rightarrow 2H_2O$$

Thermal NOx Formation: A Kinetic Example

- NOx from boilers and process heaters comprises mostly NO and very little NO2
- Consider NO formed from the high-temperature reaction of N2 and O2, referred to as thermal NOx.
- There are more than 70 steps in the sequence.
- In the case of thermal NOx, the rate-limiting step is the rupture of the N≡N triple bond by an oxygen atom:

$$N_2 + O = NO + N$$

- In turn, the nitrogen radical reacts with available oxygen as follows:

$$N + O_2 = NO + O$$

- Adding these two equations together gives the overall reaction:

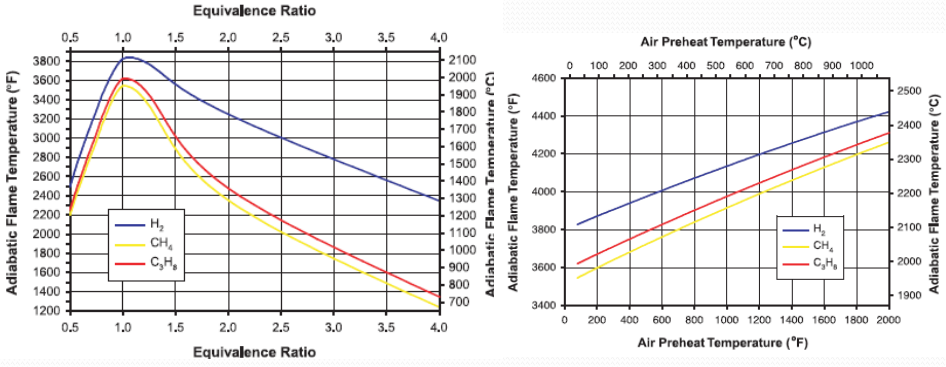
$$N_2 + O_2 \rightarrow 2\,NO$$

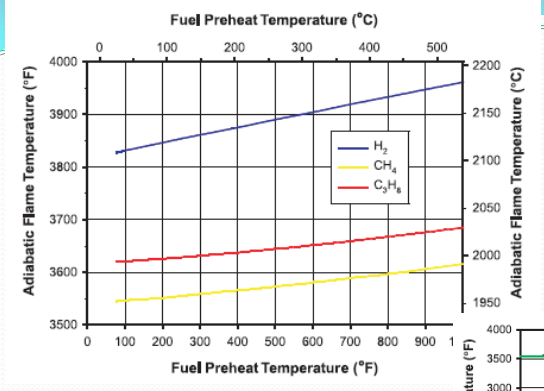
- Reaction rate:

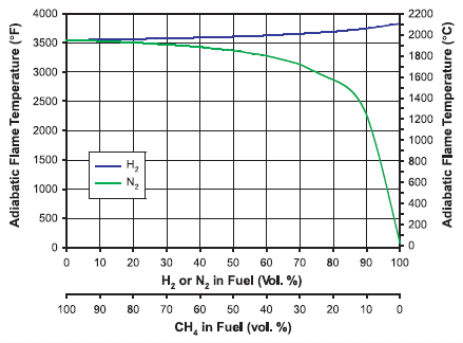
$$\frac{d[NO]}{dt} = k_f[N_2][O]$$

FLAME PROPERTIES

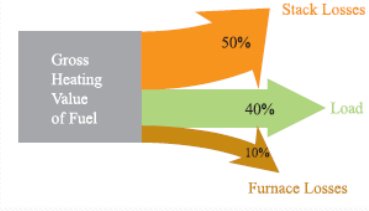
- The flame temperature is a critical variable in determining the heat transfer.
- The **adiabatic flame temperature is affected by the fuel composition**, the **equivalence rat**io, and **the air and fuel preheat temperatures**.
- The peak temperature occurs at about stoichiometric conditions (Φ= 1.0) ➔ there is just enough oxidizer to fully combust all the fuel.







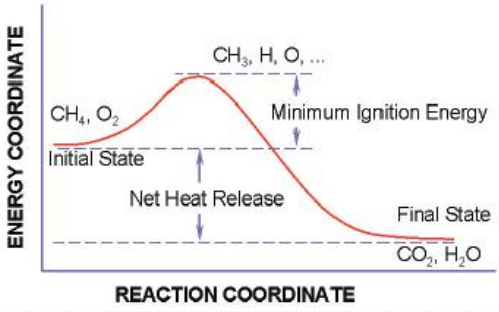
Distribution of Energy in Combustion System



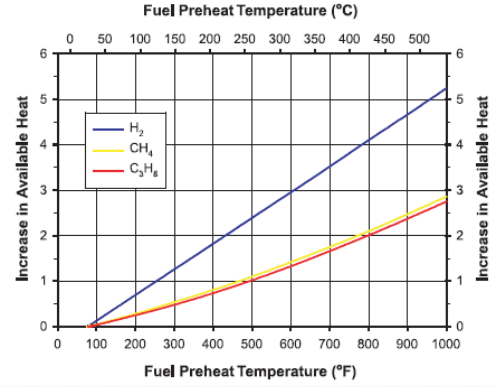
- The **available heat** in a process is defined as the gross heating value of the fuel, minus the energy carried out of the **exhaust stack** by the **flue gases**.
- However, some of that **energy will be lost** by **conduction through the heater walls**, by **radiation through openings**, by **air infiltration** that will absorb sensible energy, as well as by other types of energy losses that are dependent on the burner and heater designs and by the process operations.

Minimum Ignition Energy

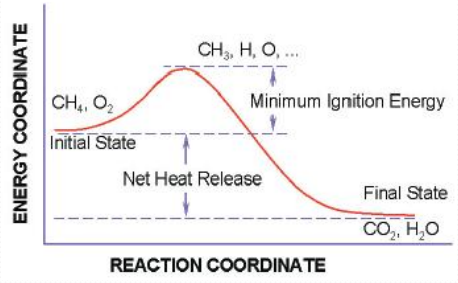
- If the **minimum ignition energy** is supplied, the reactant bonds will rupture, producing intermediate species such as CH3, H, O, etc.
- Such species are extremely reactive and recombine to form the final products, CO2 and H2O.
- Since the **net heat release is greater than the minimum ignition energy**, the reaction, once started, will continue until virtually all of the reactants are consumed



- Available heat vs. fuel preheat temperature for stoichiometric air/H2, air/CH4, and air/C3H8 flames at an exhaust gas temperature of 2000°F (1100°C), where the air is at ambient temperature and pressure.



Ignition and heat release



- Once the system reaches the minimum ignition energy, the reaction will be self-sustaining until the reaction consumes enough of the reactants.
- At that point, the reaction cannot liberate enough heat to supply the minimum ignition energy and the flame goes out.

Flammability Limits

- Suppose that fuel and air are not provided in stoichiometric proportions, but have a great excess of fuel or air. Will the flame continue to propagate if the ignition source is removed?
- That depends on **whether the fuel/air mixture has enough chemical energy to exceed the minimum ignition energy**. If not, **the flame will extinguish**.
- This leads to a lower and upper flammability limit.
- The **lower flammability limit** (fuel lean) is where fuel is insufficient to achieve the minimum ignition energy.
- The **upper flammability limit** (fuel rich) is where there is insufficient air.

TABLE 2.4 Combustion Data for Hydrocarbons

Hydrocarbon	Formula	Higher Heating Value (vapor), Btu lb_m^{-1}	Theor. Air/fuel Ratio, by mass	Max Flame Speed, (ft s^{-1})	Adiabatic Flame Temp (in air) (°F)	Ignition Temp (in air) (°F)	Flash Point (°F)	Flammability Limits (in air) (% by volume)	
Paraffins or Alkanes									
Methane	CH_4	23875	17.195	1.1	3484	1301	Gas	5.0	15.0
Ethane	C_2H_6	22323	15.899	1.3	3540	968–1166	Gas	3.0	12.5
Propane	C_3H_8	21669	15.246	1.3	3573	871	Gas	2.1	10.1
n-Butane	C_4H_{10}	21321	14.984	1.2	3583	761	–76	1.86	8.41
iso-Butane	C_4H_{10}	21271	14.984	1.2	3583	864	–117	1.80	8.44
n-Pentane	C_5H_{12}	21095	15.323	1.3	4050	588	< –40	1.40	7.80
iso-Pentane	C_5H_{12}	21047	15.323	1.2	4055	788	< –60	1.32	9.16
Neopentane	C_5H_{12}	20978	15.323	1.1	4060	842	Gas	1.38	7.22
n-Hexane	C_6H_{14}	20966	15.238	1.3	4030	478	–7	1.25	7.0
Neohexane	C_6H_{14}	20931	15.238	1.2	4055	797	–54	1.19	7.58
n-Heptane	C_7H_{16}	20854	15.141	1.3	3985	433	25	1.00	6.00
Triptane	C_7H_{16}	20824	15.151	1.2	4035	849	—	1.08	6.69
n-Octane	C_8H_{18}	20796	15.093	—	—	428	56	0.95	3.20
iso-Octane	C_8H_{18}	20770	15.093	1.1	—	837	10	0.79	5.94
Olefins or Alkenes									
Ethylene	C_2H_4	21636	14.807	2.2	4250	914	Gas	2.75	28.6
Propylene	C_3H_6	21048	14.807	1.4	4090	856	Gas	2.00	11.1
Butylene	C_4H_8	20854	14.807	1.4	4030	829	Gas	1.98	9.65
iso-Butene	C_4H_8	20737	14.807	1.2	—	869	Gas	1.8	9.0
n-Pentene	C_5H_{10}	20720	14.807	1.4	4165	569	—	1.65	7.70
Aromatics									
Benzene	C_6H_6	18184	13.297	1.3	4110	1044	12	1.35	6.65
Toluene	C_7H_8	18501	13.503	1.2	4050	997	40	1.27	6.75
p-Xylene	C_8H_{10}	18663	13.663	—	4010	867	63	1.00	6.00
Other Hydrocarbons									
Acetylene	C_2H_2	21502	13.297	4.6	4770	763–824	Gas	2.50	81
Naphthalene	$C_{10}H_8$	17303	12.932	—	4100	959	174	0.90	5.9

Note: Based largely on: "Gas Engineers' Handbook", American Gas Association, Inc., Industrial Press, 1967. For heating value in J kg^{-1}, multiply the value in Btu lb_m^{-1} by 2324. For flame speed in m s^{-1}, multiply the value in ft s^{-1} by 0.3048.

Flammability Limits for Gas Mixtures

- For gas mixtures, one can use Le Chatelier's rule to estimate flammability limits for gas mixtures.
- Because this is only an estimate, one must confirm the flammability limit of the actual mixture.
- Such experiments are relatively inexpensive and many third parties exist that can perform this kind of analysis.

$$LFL = \frac{1}{y_1\left(\frac{1}{LFL_1}\right) + y_2\left(\frac{1}{LFL_2}\right) + y_3\left(\frac{1}{LFL_3}\right) + \cdots + y_n\left(\frac{1}{LFL_n}\right)}$$

$$UFL = \frac{1}{y_1\left(\frac{1}{UFL_1}\right) + y_2\left(\frac{1}{UFL_2}\right) + y_3\left(\frac{1}{UFL_3}\right) + \cdots + y_n\left(\frac{1}{UFL_n}\right)}$$

- where LFL is the lower flammability limit, UFL is the upper flammability limit, LFLi is the LFL for species i, and UFLi is the UFL for species i.